Methyl pivalate
598-98-1 | DTXSID4027234

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 5.02e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 8.44e-01

Confidence level: 9.57e-01

Nearest Neighbors from the Training Set

Image not found
Propyl propionate
Measured: 4.56e-02
Predicted: 4.96e-02

Image not found
Isobutyl acetate
Measured: 5.42e-02
Predicted: 5.41e-02

Image not found
Propanoic acid, 1-methylethyl ester
Measured: 5.12e-02
Predicted: 5.03e-02

Image not found
Ethyl butyrate
Measured: 4.73e-02
Predicted: 5.24e-02

Image not found
Butan-2-yl acetate
Measured: 5.34e-02
Predicted: 5.96e-02